May 2004

Science & Technology REVIEW

National Nuclear Security Administration's
Lawrence Livermore National Laboratory

A Nanoscience Approach to Fighting Bioterrorism

Also in this issue:

- Securing the Nation's Seaports
- Better Algorithms Make Codes Faster
- Comparing Methods for Carbon Sequestration

About the Cover

At Livermore's BioSecurity and Nanosciences Laboratory (BSNL), researchers explore the microscopic world of living organisms, a world filled with small molecules that can damage the human body in many ways. BSNL's mission is to detect, identify, and characterize harmful molecules to help the U.S. fight bioterrorism and improve human health. On the cover, BSNL Director Jim De Yoreo demonstrates one of the powerful tools used to image and manipulate single molecules. Such tools allow researchers to gain a more realistic picture of cellular processes and architecture. The article beginning on p. 4 describes this research area and many of the recent discoveries made by BSNL researchers.

Cover design: Amy Henke

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on assuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the World Wide Web at www.llnl.gov/str.

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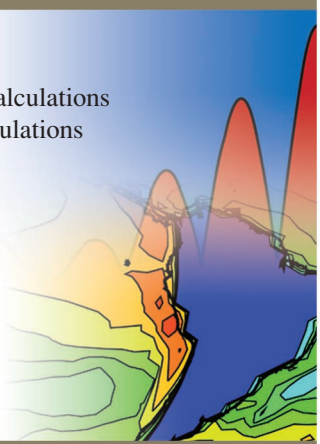
Features

Research Highlights



Departments

Genome of infectious bacterium decoded

Research teams based at Lawrence Livermore and Uppsala University in Sweden have decoded the complete genomes of separate strains of *Francisella tularensis*, a highly infectious human and animal pathogen. Also participating were researchers at Porton Down in the United Kingdom, the Swedish Defense Agency, the U.S. Centers for Disease Control and Prevention, and the Walter Reed Army Institute of Research.

"Comparing the genome sequences of the two strains will help us identify the genes, and their associated proteins, that cause one strain of *F. tularensis* to be more virulent than another," says Livermore biologist Emilio Garcia. Knowledge of the microbe's genomic sequence—the precise order of the nucleotide bases in its DNA—can improve scientific understanding of its fundamental physiology and metabolism. This knowledge also could help researchers develop more effective vaccines and better methods for diagnosing and treating tularemia.

Tularemia, or rabbit fever, is a rare but serious disease normally spread by insect bites and human contact with rabbits, prairie dogs, and other small and medium-size animals. The disease can be treated with antibiotics and is seldom fatal. However, it is highly infectious—as few as 10 organisms entering the body can induce a fever—and causes severe, long-lasting pneumonialike symptoms and various glandular and intestinal disorders. *F. tularensis* is also considered a potential bioterrorism agent.

Contact: Emilio Garcia (925) 422-8002 (garcia12@llnl.gov).

Gamma-ray bursts expel common elements

In the February 20, 2004, issue of *Astrophysical Journal Letters*, Jason Pruet, a Livermore astrophysicist, and Rebecca Surman and Gail McLaughlin of North Carolina State University report on their discovery that gamma-ray bursts are important sources of several common elements. Their findings are based on recent observations indicating that each gamma-ray burst expels about half a solar mass of readily visible radioactive nickel. After a few months, this radioactive nickel, which is moving at 40,000 kilometers per second, decays to iron. Their modeling calculations show that gamma-ray bursts also produce enormous quantities of such everyday elements as zinc, titanium, calcium, and scandium.

Gamma-ray bursts are rare—only a small percentage of dying stars produce them. But, says Pruet, these events may account for as much of some elements as all other stellar explosions combined.

Contact: Jason Pruet (925) 422-5850 (pruet1@llnl.gov).

Guide star sheds light on stellar origins

In a university–laboratory collaboration, a team of astrophysicists has observed for the first time that distant larger stars formed in flattened accretion disks just as the Sun was formed. Less massive stars, including the Sun, are believed to be formed in a swirling spherical cloud that collapses into a disk. Using the laser guide star adaptive-optics system created by Livermore scientists, the astronomers observed a strongly polarized, biconical nebula 10 arcseconds in diameter around the star LkHa 198 and a polarized jetlike feature in LkHa 198-IR. The star LkHa 233 featured a narrow, unpolarized dark lane similar to an optically thick circumstellar disk.

The team included scientists from Lawrence Livermore, the University of California (UC) at Berkeley, UC Santa Cruz, California Institute of Technology, the National Science Foundation's Center for Adaptive Optics, and UC's Lick Observatory. Results from this research were published in the February 27, 2004, issue of *Science*.

Contact: Claire Max (925) 422-5442 (maxce@llnl.gov).

Prototype containment vessel developed

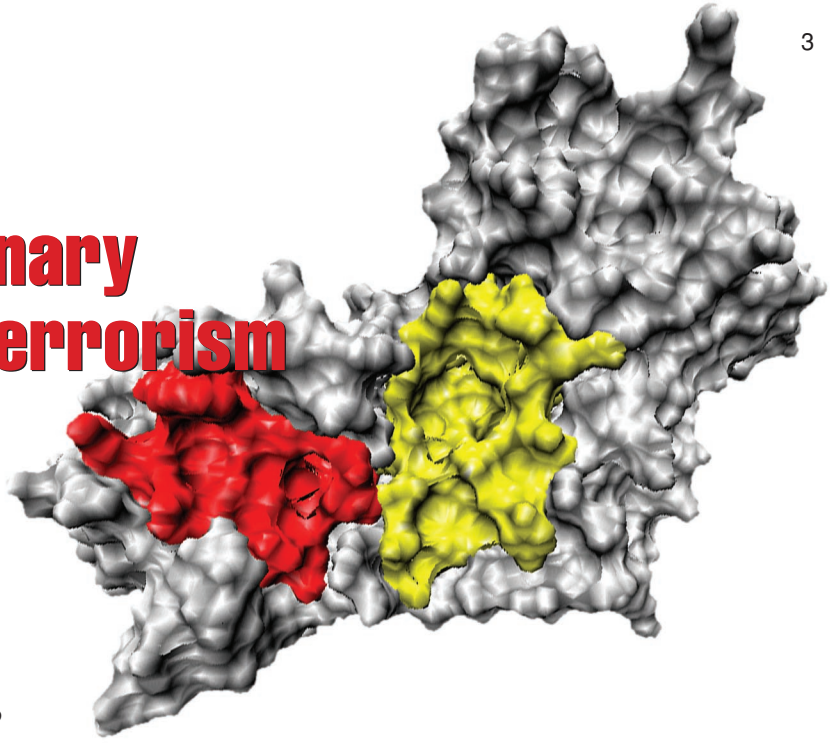
Livermore scientists and engineers have successfully tested a prototype composite containment vessel for explosive experiments. The half-scale prototype vessel, about the size of a large medicine ball, contained an internal blast from an 8-kilogram (18-pound) soccer-ball–size sphere of C4 explosive in a test at Livermore's Site 300. The new vessel is designed to accommodate the more stringent containment standards that are likely to be developed for future experiments with explosives, especially those involving nuclear material.

Low-density continuous aramid fibers, such as those used in bulletproof vests, make up the vessel's outer shell, which provides the primary structural resistance against the blast forces. An aluminum liner underneath this shell provides a sealing surface and doubles as the winding mandrel for the composite filaments. This design is stronger than steel, and radiographic measurements can be taken through the vessel wall—no ports are necessary.

The team's work is part of a joint project with Los Alamos National Laboratory to develop a full-size (2-meter-diameter) windowless firing vessel that can completely contain a cased explosive with up to 0.04 metric ton (80 pounds) of TNT equivalent.

Contact: John Pastrnak (925) 422-8403 (pastrnak@llnl.gov).

A Multidisciplinary Attack on Bioterrorism



THE most promising scientific fields of the new century are emerging at the boundaries between historically separate disciplines. This is especially true in the fields of chemistry, biology, materials science, and physics. For example, chemists are using atomic force microscopes to reveal the structure of viruses, and physicists are developing sensors that can detect minute quantities of airborne pathogens. Meanwhile, extraordinary breakthroughs in nanoscience—the study of materials at a billionth-of-a-meter resolution—are giving scientists the ability to manipulate individual molecules in their natural environment and develop complex molecular machines the size of microbes and even smaller.

As described in the article beginning on p. 4, Livermore's BioSecurity and Nanosciences Laboratory (BSNL) has put together teams of chemists, biologists, physicists, and engineers to pursue research at the intersection of the physical and biological sciences. The BSNL research teams, composed of staff from Chemistry and Materials Science (CMS) and partnering directorates at Livermore, are using some of the most advanced imaging and analytical instruments in the nation.

Livermore has the opportunity—and the duty—to strengthen homeland security by helping prevent a bioterrorist act and strengthening the nation's response should one occur. BSNL's most important mission is to develop new ways to detect, image, and understand bacterial and viral pathogens that might be used in a bioterrorist attack. As the article details, several BSNL scientists are also analyzing the changes in blood serum proteins as a way to provide an early warning system for the onset of disease resulting naturally or from terrorist agents.

The knowledge and techniques gained from BSNL research projects are sure to improve human health and environmental remediation efforts by shedding new light on how microbes function and are structured. I also expect that the technology being developed for new biodetectors and sensors will be adapted to advance the Laboratory's long-standing missions in defense and stockpile stewardship, especially in monitoring changes in the nation's nuclear stockpile.

BSNL's organization and research efforts match well with the needs of the Department of Energy's (DOE's) Genomics:GTL Program (previously called Genomes to Life) for understanding the proteins encoded by the human genome. This major initiative, which follows the Human Genome Project, notably calls for well-integrated, multidisciplinary research teams. We believe that by partnering with Livermore's Biology and Biotechnology Research Program Directorate, BSNL scientists can make an important contribution to the national Genomics:GTL Program. BSNL researchers are already building intracellular probes for tracking proteins and studying their interactions with other proteins.

One of the most exciting attributes of BSNL is the sizable number of young researchers. We have tried to institute a supportive environment within BSNL for the brightest young scientists we can find. We're providing them with the most advanced resources to help them flourish as they explore new ideas that other institutions might consider too risky to support. The quality of our research environment is proving to be a magnet for university collaborations and for recruiting outstanding new graduates. Several Lawrence fellows have joined BSNL, plus we have young researchers completing their Ph.D.s and a growing number of college summer students. Many students working at BSNL are being trained in the physical sciences but are interested in solving challenging problems in biology.

We're reaching out to potential sponsors for BSNL projects, such as DOE's Office of Biological and Environmental Research within the Office of Science and the National Institutes of Health. Our research is extremely relevant to these federal agencies. We're also strengthening partnerships with other Livermore directorates whose scientists have skills that complement those in CMS.

BSNL scientists are using their skills and creativity and Livermore's unmatched resources to make a significant contribution to the war on terrorism. I am confident that our multidisciplinary approach will also produce substantial gains in medicine, environmental remediation, and scientific understanding of the machinery of life.

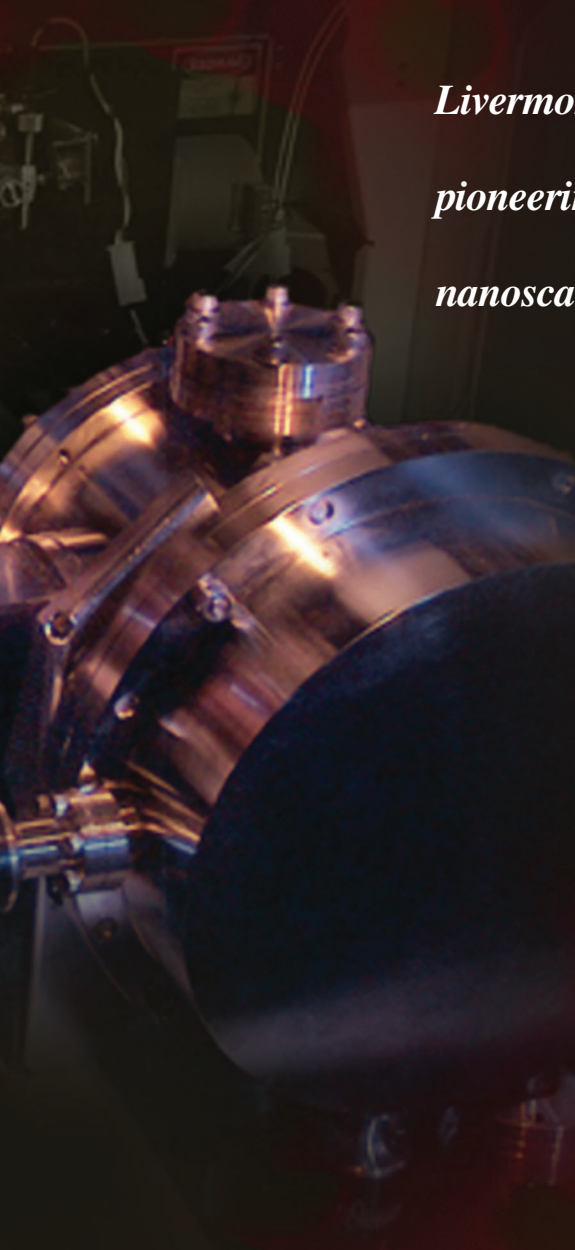
■ Tomás Díaz de la Rubia is associate director of Chemistry and Materials Science.

Life at

Sharon Shields, a chemist at Livermore's BioSecurity and Nanosciences Laboratory, uses a time-of-flight mass spectrometer to identify the proteins found in blood serum. These proteins are produced in response to the presence of pathogens.

the Nanoscale

Livermore's BioSecurity and Nanosciences Laboratory is pioneering new ways to detect pathogens and biomolecules at the nanoscale level and study how they function.



UNTIL recently, national security was synonymous with guns, tanks, and planes. Increasingly, however, the notion of security, especially homeland security, demands a broader meaning that includes ways to quickly detect and identify biological pathogens that might be unleashed by terrorists. Such pathogens could threaten urban population centers, crops, and livestock.

Livermore's BioSecurity and Nanosciences Laboratory (BSNL) is proving itself a national asset in the fight against bioterrorism by discovering new methods to detect, identify, image, and understand pathogens such as viruses, bacteria, and their spores. The research findings are also helping improve human health by providing a better understanding of pathogens and molecular machines such as DNA and proteins. In addition, BSNL researchers are contributing to the Department of Energy's Genomics:GTL Program, the follow-on effort to the Human Genome Project. The goal of Genomics:GTL (formerly called the Genomes to Life Program) is to understand the function of proteins and how they form the machines that drive the cells. Such information will help scientists better understand the complex biochemical activity of microbes.

BSNL's 62 researchers are drawn principally from Livermore's Chemistry and Materials Science Directorate, with significant contributions from the Biology and Biotechnology Research Program (BBRP); Engineering; Energy and Environment; Nonproliferation, Arms Control, and International Security; and Physics and Advanced Technologies directorates. More than half of the researchers are under 35 years old. "From the start, we adopted a strategy of investing in young talent, both from around the Laboratory and from scientists around the nation who are just starting their careers," says BSNL Director Jim De Yoreo.

The center has attracted four Lawrence fellows, who are some of the most sought after young Ph.D.s in the world. In addition, 27 students have worked with

BSNL scientists over the last three years; 11 student employees are currently doing their thesis work at BSNL. De Yoreo says the many young people create an environment where scientists do not hesitate to try new approaches and seek breakthroughs at the risk of failure.

Multidisciplinary research teams work at what De Yoreo terms the intersection of biology, chemistry, and materials science. Principal research areas are protein analysis and systems biology, bioaerosol science, molecular recognition chemistry, physical and chemical pathogen signatures (detection techniques), nanofabrication of devices, and cellular- and molecular-scale measurements.

A Natural Synergy

Founded in 1999 as the BioSecurity Support Laboratory, BSNL was reorganized in 2003 to increase its focus on what De Yoreo calls the "natural synergy" between nanotechnology and new frontiers in biological research. BSNL researchers work to exploit this synergy in three areas: sensing viruses, bacteria, and toxins; fabricating materials from the bottom up; and understanding the assembly and performance of protein machines and cellular systems.

Nanoscience takes its name from the nanometer, which is a billionth of a meter. BSNL researchers work on the nanoscale, or single molecule scale, to understand the organization of molecular complexes that make up most spores, viruses, DNA, or proteins—a level that provides unprecedented detail. (See *S&TR*, December 2001, pp. 12–19.)

At the nanoscale, experimental results can be viewed only with the most powerful imaging techniques, such as atomic force microscopy (AFM), confocal optical microscopy, and nano secondary-ion mass spectrometry. The two microsopy techniques can even image and manipulate single molecules, allowing researchers to study a molecule's structure and function. BSNL researchers' emphasis on single molecules differs greatly from that of traditional biological researchers, who examine beakers full of material and infer the actions of individual molecules.

Although electron microscopes have greater resolution, specimens must be frozen and covered with a metal film prior to imaging. With the optical methods used at BSNL, researchers can probe live cells to gain a much more realistic picture of their functioning and architecture.

Supporting some of the research is computer simulation. For example, BSNL scientist Andrew Quong used the Laboratory's ALE3D code to develop three-dimensional (3D) models that examine how epithelial cells communicate with each other. The simulations show strong agreement with experiments. (See *S&TR*, January/February 2003, pp. 15–18.)

The researchers are experts at synthesizing nanostructured materials such as artificial membranes with nanometer-size pores, microfluidic channels that guide the flow of single molecules for analysis, surfaces with nanometer-scale chemical patterns, and chemical compounds that recognize—or bind to—specific targets such as toxin molecules. Synthesis methods include using cells as chemical factories as well as traditional small-molecule techniques that can produce synthetic high-affinity ligands, which bind to pathogens and render them harmless. (See *S&TR*, June 2002, pp. 4–11.)

The First Signs of Disease

One of the most powerful tools used by BSNL scientists is the mass spectrometer, a device that measures the mass of individual molecules to precisely identify them. The instrument is being used to understand how cells respond when exposed to pathogens. The research is part of a pathomics project funded by Livermore's Laboratory Directed Research and Development Program. The term pathomics was coined by co-principal investigator Ken Turteltaub, a molecular biologist in BBRP. It is the science of applying proteomics, the study of proteins, to the discovery of certain proteins whose appearance or increase in concentration indicates a particular pathogen is present.

BSNL chemist Henry Benner says the research team ultimately wants to understand how individuals respond to pathogens, particularly those that bioterrorists might use. Such an improved understanding could lead to detection systems that identify an attack or disease outbreak before the first symptoms appear. "Our goal is to develop a technique that would analyze the proteins in a sample of blood serum and quickly detect the presence of a pathogen long before someone felt ill."

The project involves biologists, physicists, chemists, engineers, and computer scientists and uses some of the most sensitive mass spectrometers in the world. Says Benner, "This type of big, integrated project would be difficult to duplicate anywhere else."

The researchers are focusing first on human and animal serum proteins that are produced in response to vaccinia virus, the surrogate for smallpox virus. They are also collaborating with other institutions to determine how rodents can be used as model systems for human biochemical changes. In addition, they are studying how cell cultures can model the progression of a pathogen-caused disease.

Benner and chemists Sharon Shields and Chris Bailey have developed a liquid chromatography and mass spectrometry analysis system for characterizing plasma proteins in serum. Because most intact proteins are too large for the mass spectrometer to analyze, the team first applies an enzyme to the serum, which cuts each protein into about 50 chunks per molecule. The liquid chromatograph then separates and ionizes the protein chunks before they enter the mass spectrometer.

Detecting 10,000 Proteins

Benner notes that human blood serum can contain up to 10,000 different proteins, many of which are unknown. "With mass spectrometry, we analyze everything that's in the serum. We really don't need to identify every protein, although we'd like to eventually have that information. All we're looking for is a complex pattern—a series of mass spectrometry peaks—that corresponds to someone who is in the earliest stages of bacterial or viral attack and another pattern that corresponds to a healthy individual."

Almost certainly, different pathogens will produce different patterns. In this way, the researchers hope to accumulate a library of mass spectrometry patterns that identify specific pathogens. In addition, they must determine the extent to which various serum proteins vary in both normal and diseased individuals.

Another goal for the research team is to discover one or a few proteins that are a dependable signature for a pathogen's presence. This type of pathogen signature, based on proteins, differs from more traditional DNA-based signatures developed by Livermore researchers. (See *S&TR,* April 2004, pp. 4–10.)

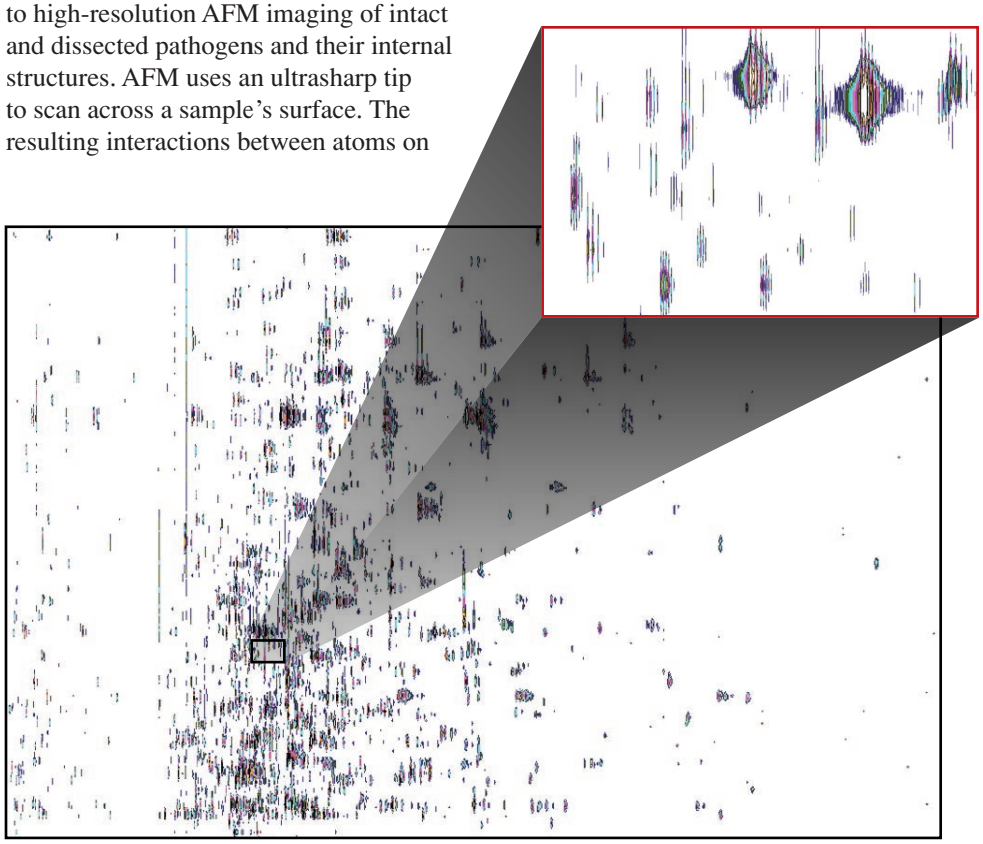
When perfected, the BSNL mass spectrometry technique would be valuable for detecting a bioterrorist attack, a natural outbreak of infectious disease, and even types of cancer. Another potential application is continual monitoring of the nation's blood supply. Patients receiving radiation treatment could also benefit from the technology because different mass spectrometry patterns would uniquely indicate damage to certain organs. A related project, led by scientists in BBRP and Livermore's Glenn T. Seaborg Institute, is using biomass spectrometry of blood serum to determine whether someone has been exposed to a dirty bomb—a crude nuclear device designed to cause widespread dispersal of radioactive materials.

Seeing Pathogens at the Nanoscale

Identifying and characterizing proteins that reside on the surface of human pathogens and that form their internal structures is critical to understanding how pathogens cause disease. Such information is also essential for developing vaccines and detectors for both medicine and biodefense. However, despite decades of study, scientists still have a poor understanding of many pathogens' structural properties. Common tools such as x-ray crystallography and electron microscopy often cannot be used because of some pathogens' large size, heterogeneity, and lack of symmetry.

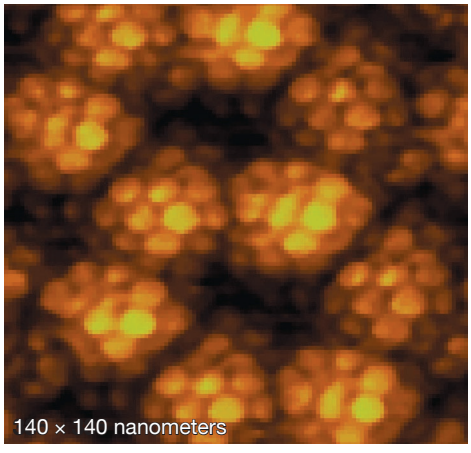
As a result, BSNL scientists have turned to high-resolution AFM imaging of intact and dissected pathogens and their internal structures. AFM uses an ultrasharp tip to scan across a sample's surface. The resulting interactions between atoms on the surface of the sample and those on the AFM tip are used to construct a high-resolution image of the surface topography.

BSNL chemists Alexander Malkin, Marco Plomp, and others are using AFM to image the proteins of intact human viruses and bacterial spores. They are focusing on bioterrorist threat surrogates such as the vaccinia virus, a laboratory model for smallpox virus. Vaccinia virus is one of the largest and most complex human viruses. The researchers are also studying several species and strains of innocuous *Bacillus* spores to understand the spore structure and function of *B. anthracis,* the agent of inhalation anthrax.



BSNL researchers use liquid chromatography to separate and ionize chunks of protein in a sample of blood serum and then analyze them with a mass spectrometer. The researchers hope to detect a pattern of mass spectrometry peaks (inset) that correspond to someone in the earliest stages of a particular bacterial or viral attack and another pattern that corresponds to a healthy individual. Each group of spots represents a single protein fragment.

For more than eight years, the researchers studied the molecular-scale mechanisms of crystallization for several types of proteins, viruses, nucleic acids, and ribosomes. Then using AFM, they imaged the high-resolution structure of these large ensembles of macromolecules. In work on agricultural viruses, Malkin imaged for the first time the structure of a small virus's capsid—the protein shell covering the viral genome—under physiological conditions. Image resolution approached an unprecedented 2 nanometers and clearly revealed the individual protein capsomeres that make up the capsid. (See the top figure below.) Malkin has demonstrated that viruses from different but closely related virus families can be differentiated by AFM on the basis of their capsid structure.



Atomic force microscope image of a crystalline array of turnip yellow mosaic viruses reveals the capsid structure, which can be resolved at high resolution.

Viral and Spore Structures

The scientists also imaged the Herpes Simplex Virus-1, one of the most widespread human viruses. This work demonstrated for the first time that the internal topography of viruses could be revealed by AFM using chemicals and enzymes to degrade particles from the outside to the inside, revealing each layer of the virus. Images showed the intact virus, the underlying capsid and its capsomere components, and finally, extrusion of viral DNA.

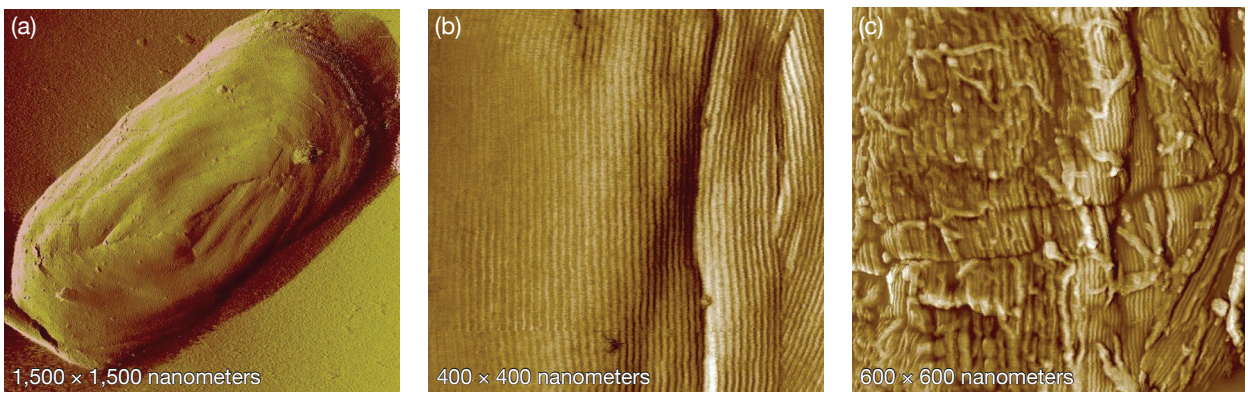
Evaluating the response of pathogens to the environment is important for understanding pathogen lifecycles and could help scientists develop detection systems and decontamination procedures. The researchers have visualized both hydrated and dehydrated samples of vaccinia virus. AFM images show that the surface of the hydrated form bristles with about 30-nanometer protein protrusions that had never been previously described for pox viruses. A membrane surrounds the viral core, which consists of 16-nanometer-diameter filaments containing double-stranded DNA. AFM visualization of intact viruses and their internal structures allows researchers to model the complex internal architecture of a large human virus.

Malkin and Plomp recently began visualizing bacterial spores. They resolved the surface structure of a *B. atrophaeus* spore coat and found that, in hydrated form, the top surface layer consists of regular arrays of rodlike crystalline structures that fold when dehydrated. (See the figure below.) In a study of two other *Bacillus* species, they found striking differences in spore structure. One species (*B. thuringiensis*) had an outer spore coat formed by a hexagonal honeycomb crystalline structure, whereas the other (*B. cereus*) had an outer rodlike structure and an underlying honeycomb structure.

The researchers are also pioneering a new approach called AFM-based immunolabeling. In this work, they use monoclonal antibodies synthesized to bind to targeted viral and spore proteins. The research is conducted in collaboration with scientists from the Oakland Children's Hospital Research Institute and the National Institute of Allergy and Infectious Diseases.

The mapping of surface proteins using monoclonal antibodies is a powerful tool for examining the surface topology of pathogens. Each bound monoclonal antibody defines one specific site on the antigen's surface. In this way, AFM can determine the location of proteins on a pathogen's surface—information that will

These images resolve the shape and surface features of a *Bacillus atrophaeus* spore. (a) A hydrated spore is magnified in (b), showing a surface consisting of arrays of rodlike structures that fold when dehydrated (c).



help scientists develop vaccines, detection systems, bioforensic methods, and decontamination procedures.

New Kinds of Sensors

One of BSNL's most important research goals is developing fast, sensitive, and accurate instruments to detect and identify a wide range of pathogens. In the area of airborne pathogen detection, Livermore researchers have worked with colleagues at the University of California (UC) at Davis to develop the bioaerosol mass spectrometer (BAMS). BAMS combines advanced laser desorption and ionization techniques with mass spectrometry, and it is two to three times more sensitive than other laser ionization techniques. In addition, the response time for BAMS is fast—it can identify a single airborne particle in about 100 milliseconds. (See *S&TR*, September 2003, pp. 21–23.)

Other researchers are working to shrink pathogen sensors to the size of a semiconductor chip for bioterrorism and health-care applications. BSNL physical chemist Alex Noy and graduate student Alex Artyukhin are developing a new kind of biosensor that is based on a lipid-coated nanotube, the first ever manufactured. In effect, the sensor is a tiny but mechanically resilient "molecular wire" designed to detect pore-forming bacterial toxins. These toxins, which are large proteins, are secreted by the bacteria and insert themselves into outer membranes of host cells. The 2-nanometer-wide holes created by the proteins rupture the cell and kill it.

To construct the biosensor, the researchers start with a carbon nanotube—a rolled-up, single layer of graphite. If the tube is rolled in a specific orientation, it becomes a semiconductor, a material that allows electrons to flow under certain conditions. Because of their electrical properties, semiconductors make excellent sensors.

With the help of microfabrication expert Olgica Bakajin, the researchers coat the nanotubes with a 5-nanometer-thick, dual-layer membrane made of phospholipids. The result is an insulated wire that mimics a cell membrane.

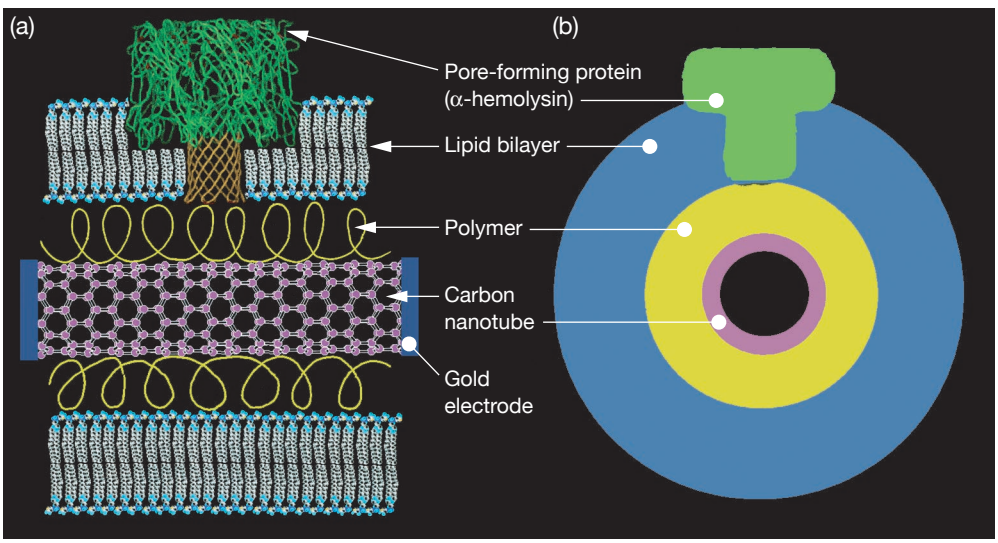
"Our idea was to construct something like a shielded cable that would be a good electrical detector," says Artyukhin. With electrodes attached to both ends of the nanotube and a voltage applied, the minuscule sensor can detect pathogen toxins that typically puncture a hole in a cell membrane or an artificial one. Any pathogen toxins in the immediate environment would insert themselves into the membrane. The punctures they create would allow ions to rush in, touch the bare nanotube, and immediately change the voltage.

The researchers recently added a polymer layer between the carbon nanotube and the lipid bilayer, to confer electrical stability and increase the tube's diameter. Many proteins require more room to function when they protrude through a membrane. The polymer layer can be reapplied to make several layers, each 1 nanometer thick. The researchers are experimenting with a five-layer nanotube.

Once perfected, the biosensor would be cheap to manufacture because it could be fabricated by the thousands, much like semiconductor chips in clean rooms. "Our biosensor is extremely simple," says Artyukhin. "It doesn't need lasers or other sophisticated equipment to function." The device would be ubiquitous and function as a "biological smoke detector."

A Close Look at Packaged DNA

AFM is central to a research effort headed by Noy that examines how DNA is packaged



A new type of biosensor is based on a lipid-coated nanotube: (a) longitudinal and (b) transverse sections. The sensor is designed to detect bacterial toxins such as the protein α-hemolysin, which pokes 2-nanometer-wide holes in cell membranes. The biosensor starts with a rolled-up carbon nanotube that is coated with a layer of polymer molecules and then a bilayer of phospholipids that mimic a cell membrane. With electrodes attached to both ends of the nanotube and a voltage applied, the minuscule sensor can detect pathogen toxins that puncture a hole in the membrane.

inside the cell nucleus so that it is a small fraction of its uncoiled size. He cites famed baseball player Yogi Berra, who once said, "You can observe a lot just by watching."

"Proteins mediate DNA packaging in all organisms," says Noy. Packaging protects DNA from physical damage and from free radicals, which are extremely reactive molecules. Different species package DNA differently. For example, mammalian sperm DNA is wrapped into dense toroids, like a pile of rope. But the mechanisms of how different proteins package DNA into distinct shapes are poorly understood.

Noy is focusing on the role of AbF2, a protein in yeast mitochondria—the cellular organelles that produce energy. AbF2's role is to "scrunch" DNA into a much more compact size. In collaboration with graduate student Ray Friddle and researchers at UC Davis, Noy has acquired AFM images of the DNA–AbF2 molecule. The images (below) show how the AbF2 binds to DNA and reveals the DNA–protein complex making repeated bends of 102 degrees.

"We then wondered whether the bends were important to compaction," Noy says. To find the answer, he constructed a computer model of the molecule, including the 102-degree bends. The model fit perfectly with data obtained from the images and showed that the bending indeed causes compaction. "When we put certain bends into DNA, it naturally folds into a compact shape," he explains.

An important lesson from this research is that studying and imaging a single molecule yields significant rewards. "When we use the single molecule technique," says Noy, "we get both binding information and the binding mechanism—the 102-degree bends. Traditional methods give binding information and then force us to deduce the mechanism."

Every new piece of data about a protein's structure and function helps efforts to detect, identify, and treat disease, says Noy. "We need to know what bad microbes do. The first rule is 'Know Your Enemy.'"

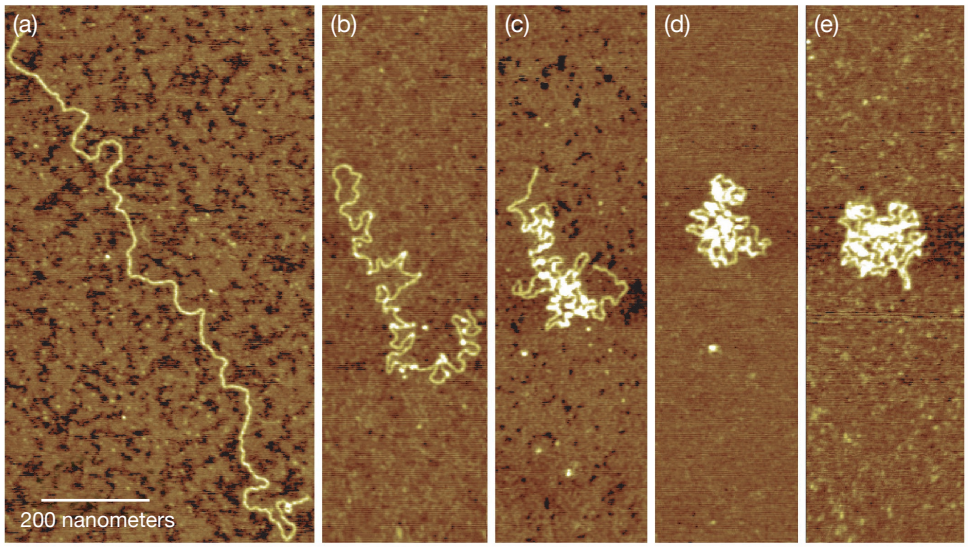
Probing Inside a Cell

BSNL physicist Thomas Huser and his colleagues Chris Hollars, Chad Talley, Anthony Esposito, and Stephen M. Lane have developed optical probes that enable nondestructive characterization and identification of cells and their functions at the nanometer scale. These probes use Raman scattering—the inelastic scattering of light by molecular bonds. Raman scattering is one of the few optical techniques that can identify a molecule by observing its distinct vibrational fingerprints as the molecule scatters laser light. (See the top figure on p. 11.) It also provides a more accurate representation than common fluorescent labeling of biomolecules. "With fluorescent techniques, we have to introduce fluorescent molecules that attach to the biomolecules of interest," says Huser. "Raman is the intrinsic signal from the native material."

He uses the confocal microscope, which is based on a fluorescence microscope augmented with a pinhole that limits the volume being probed and thus decreases background noise. The confocal microscope efficiently collects the scattered light emitted from molecules that have been excited by laser light. With this technique, Huser can perform Raman spectroscopy on single cells and look for differences between them.

The one drawback is that Raman spectra are quite weak. To increase the brightness and resolution of Raman-scattered light, Huser attached nanometer-size gold crystals to molecules or cells. The method, known as surface-enhanced Raman spectroscopy, increases the signal by a factor of a quadrillion (1×10^{15}) and vastly improves the sensitivity of the measurements.

Gold nanoparticles about 50 nanometers in diameter serve as tiny detectors that "report" on the environment they're in through Raman scattering. The particles are covered with molecules of mercaptobenzoic acid. Depending on pH, this molecule changes its Raman spectrum. "In essence, we've created an intracellular



(a–e) Progressive images from atomic force microscopy show the compaction of DNA in yeast caused by a protein called AbF2.

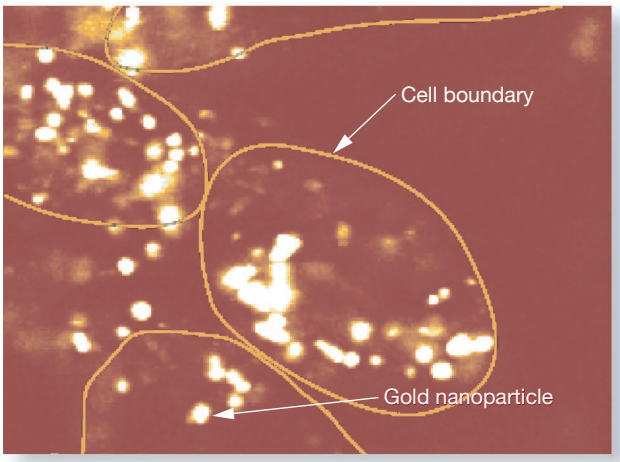
pH nanosensor that reacts to changes in its chemical environment," says Huser. If a cell undergoes changes as a result of external stimuli, its pH will usually change in response.

One possible application of this technique is studying the pH of cancer cells. Although tumors tend to be more acidic than normal tissue, the pH inside individual cancer cells is still mostly unknown. "We want to compare the pH of cancer cells to the exterior cell environment and to normal cells," Huser says. "We'd also like to see if cancer cell pH changes in response to different chemotherapy agents." Another possibility is to place the nanoparticles just outside the cells to signal the presence of certain proteins belonging to pathogens.

Huser and his colleagues are applying their expertise in a Genomics:GTL project, using nanoprobes to study how microbes clean up the environment by digesting toxic molecules. "Microbiologists would like to obtain much more detailed information about how some microbes assimilate toxic materials," he says.

Huser and Hollars are also part of a new effort, headed by Bailey, to study a class of mysterious proteins called prions. When misfolded, prions can attack healthy cells. Prions cause mad cow disease, technically known as bovine spongiform encephalopathy, and humans can contract a similar form, known as variant Creutzfeldt–Jacob disease. In sheep, prions cause a degenerative disease called scarpie.

In collaboration with the U.S. Department of Agriculture, the team is developing techniques to look for prions in sheep blood serum. One approach is to add fluorescent molecules that would bind to any prions. The serum is then run through microfluidic channels that are 100 micrometers wide, 500 micrometers long, and 0.5 micrometer deep. An optical microscope, sensitive to fluorescence, would detect any prions.



Scientists are using gold particles measuring 50 nanometers in diameter as cell pH sensors. The particles are coated with molecules of mercaptobenzoic acid, which changes its Raman spectrum in response to changes in the chemical environment.

BSNL chemist Chad Talley (left) and physicist Thomas Huser use a fluorescent microscope with a wide field of view to image single molecules.

Meeting the Vision

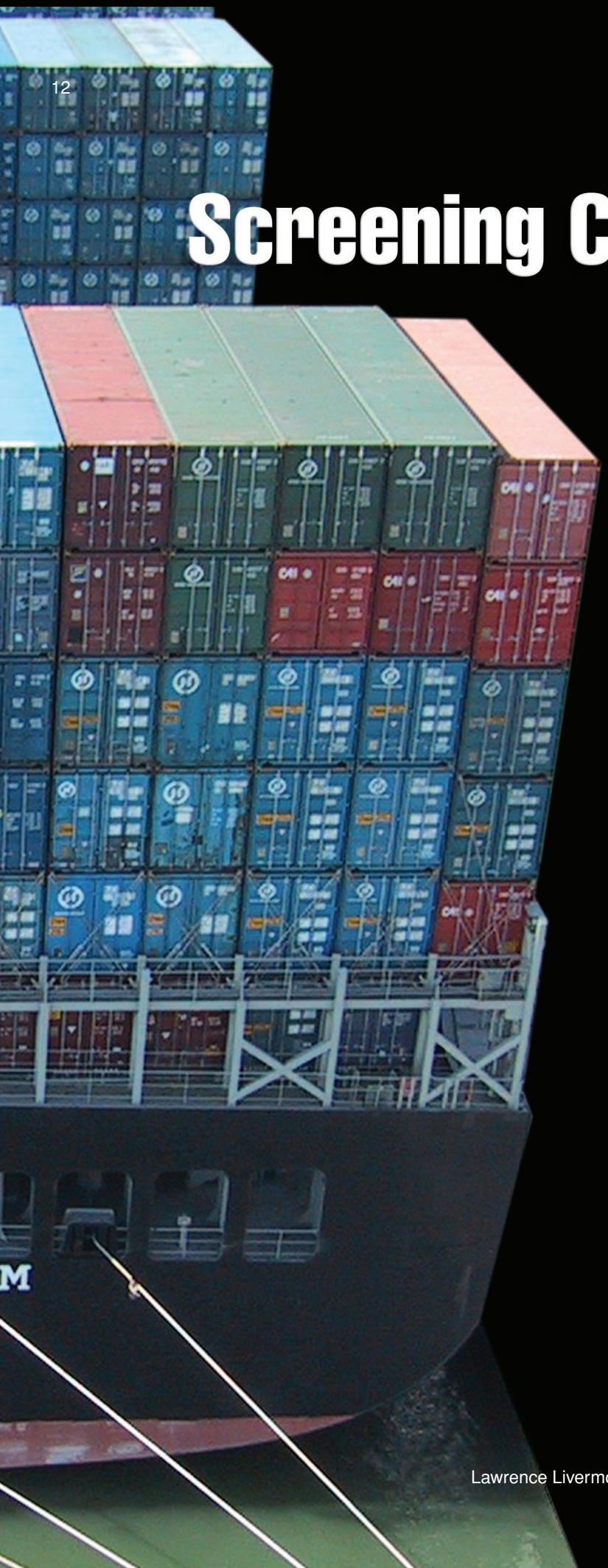
By any standard, says De Yoreo, BSNL is meeting its goals to become a formidable resource for advancing national biosecurity, improving human health, and understanding the molecular machinery of life. Increasing funding from sponsors, a growing number of publications in major peer-reviewed journals, and deepening scientific understanding of pathogens and biomolecules all speak to its success. The next few years should bring even greater understanding of life processes at the nanoscale.

—Arnie Heller

Key Words: atomic force microscopy (AFM), biodefense, BioSecurity and Nanosciences Laboratory (BSNL), bioterrorism, DNA, Genomics:GTL Program, nanoparticles, nanoscale, nanotube, pathogens, pathomics, prions, proteomics, signatures, smallpox.

For further information contact Jim De Yoreo (925) 423-4240 (deyoreo1@llnl.gov).

Screening Cargo Containers



Livermore scientists are developing a system to search for weapons and fissile materials that terrorists might hide in cargo shipped to U.S. seaports.

EACH year, some 48 million cargo containers move between the world's ports. More than 6 million of these enter the U.S., but only about 2 percent are opened and inspected when they arrive at U.S. seaports. The West Coast ports of Los Angeles–Long Beach, Oakland, and Seattle alone process 11,000 containers per day, or about 8 containers per minute.

Because of this high traffic volume, U.S. seaports are especially vulnerable to a terrorist attack. Illicit radioactive materials could be hidden in any one of the cargo-filled containers that arrive at U.S. ports. Yet, searching every shipment would bring legitimate commercial activities to a halt. Improving security at U.S. ports is thus one of the nation's most difficult technical and practical challenges because the systems developed for screening cargo must operate in concert with ongoing seaport activities.

Working at this intersection of commerce and national security, Lawrence Livermore researchers are applying their expertise in radiation science and detection to develop improved technologies for detecting hidden radioactive materials. One new technology being designed and tested at the Laboratory is a neutron interrogation system for cargo containers. This system will quickly screen incoming shipments to ensure that nuclear materials such as plutonium and highly enriched uranium (HEU) are not smuggled into the U.S.

Balancing Security and Commerce

The Livermore system would bathe suspicious containers in neutrons to actively search for nuclear materials. A truck carrying a container laden with suspicious cargo would be towed over a generator that would bombard the container with neutrons. It would then be towed through an array of detectors, much like driving through a car wash. If the

to Remove a Terrorist Threat

neutrons encountered any fissile material shielded and hidden among the container's contents—whether produce, clothing, electronics, lumber, automotive parts, or other consumer goods—the interaction would induce tiny fission reactions. These reactions would produce the telltale delayed gamma rays of nuclear materials, which would be picked up by the detectors.

The Livermore system is not intended to screen every container entering a U.S. seaport. Instead, it will be used on the suspect cargo identified by screening procedures, such as radiography or passive radiation inspection, that show some of a container's contents.

The 19-member project team draws on the talents of personnel from Livermore's Engineering Directorate as well as the Physics and Advanced Technologies; Chemistry and Materials Science; Safety and Environmental Protection; Nonproliferation, Arms Control, and International Security (NAI); and Computation directorates. "To some approximation, we work like a soccer team of 8-year-olds," says project leader Dennis Slaughter, technical director of Livermore's 100-megaelectronvolt (MeV) electron linear accelerator (linac). "By that, I mean we all follow the ball. There are no established positions. Everyone 'turns to' the urgent task, and we all help each other without disciplinary distinctions."

Originally funded by Livermore's Laboratory Directed Research and Development effort, the detection project was picked up by the Department of Energy (DOE) in 2003 and is now supported by the Department of Homeland Security (DHS). The Livermore team is focused on developing a system that is not only reliable but also commerce-friendly.

"We want a system that can detect small targets of nuclear material—about 5 kilograms of HEU and 1 kilogram of plutonium—with low error rates of about 1 percent false positive and false negative," Slaughter says. "This system would permit rapid scanning so it wouldn't disrupt commerce. Our goal is to complete the scan and report in about a minute."

An Active Interrogation System

Slaughter and his colleagues consider active interrogation to be the most promising option for detecting HEU in containers. Even moderate amounts of shielding make it difficult to passively detect radiation emanating from hidden sources. The high-energy, gamma-ray signature produced when neutrons interact with nuclear material is unique, so the liquid scintillation detectors can readily distinguish it from the signature for normal background radiation.

The neutron scan would pose few risks to cargo. Most residual radioactivity would dissipate within seconds after the scan. In the team's experiments, radiation dose rates were low.

The team is also working to minimize potential risks to the people who will operate the equipment. The project goal is to limit radiation exposure to the normal allowable doses specified in federal standards for the general public. "Because people might be inside a container during irradiation," says Slaughter, "we want the radiation dose to be too small to cause harm."

Slaughter hopes to see such a system as a regular part of cargo container security at U.S. ports. Eventually, it might also be used at foreign ports to scan containers before they are loaded aboard U.S.-bound ships. Since 2002, the Livermore team has done considerable work related to basic science and engineering of the system, developing the detector and establishing requirements for the neutron generator. Research has been conducted at Livermore and at the 88-inch cyclotron at Lawrence Berkeley National Laboratory (LBNL). The team's timetable is to build a research prototype and evaluate it in a laboratory setting during 2005 and field a vendor prototype at a container port in 2006.

Detecting the Gamma-Ray Signature

Use of a high-energy, gamma-ray signature to detect nuclear materials in containers was proposed by Stanley Prussin, a professor of nuclear engineering at the University of California (UC) at Berkeley, and Eric Norman of LBNL. Prussin, now the chief scientist for the cargo container project, has long consulted with the Laboratory's NAI Directorate. He became involved with the cargo container effort in the summer of 2002 while on sabbatical at Livermore to work on an unrelated project.

Prussin was familiar with Slaughter's work and attended a meeting at which modelers discussed the container effort. He says, "It didn't take too long for me to become convinced that, under their defined worse-case condition, we ought to take another look at the technique they were modeling."

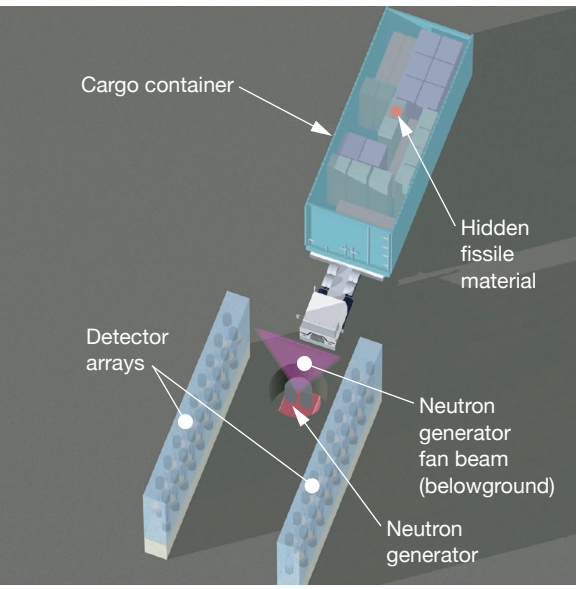
Rather than high-energy gamma rays, the Livermore team originally considered a system that counted delayed neutrons emitted by neutron-induced fission. Delayed neutrons are emitted from a fraction of a second to a few minutes after fission and have lower energies than the fast prompt fission neutrons. Although delayed neutrons can be a reliable indication of nuclear materials, their yield is low.

Prussin noted a difficulty with using delayed neutrons: Hydrogenous cargo—fruits and vegetables, canned meats, wood, plastics—can absorb the short-lived

neutrons and thus might interfere with the delayed neutron count.

"Any system we develop must look for fissionable materials that will be well shielded," says Prussin. "If the material is shielded by hydrogenous material, the probability for the delayed neutrons to actually escape from the container into an external detector is very small. In the U.S., we import almost everything under the sun, and many of those imports are hydrogenous."

Instead of the delayed neutron count, Prussin suggested the team measure the gamma rays emitted. Fission products make numerous gamma rays that have comparable decay characteristics of delayed neutrons. Yet, says Prussin, the probability of the neutron-induced gamma rays escaping from the container through hydrogenous material is about 1,000 times greater than it is for delayed neutrons.



The design for the detector system calls for a belowground neutron generator that would bathe containerized cargo with neutrons. Interaction of the neutrons with fissile material inside the container would produce fission, followed by delayed gamma rays detected by an array of liquid scintillators as the container moves through the system.

In 2003, Prussin and Slaughter worked with Norman to arrange for a series of experiments, funded by DOE's Office of Science, at LBNL's 88-inch cyclotron. The first experiment was conducted using a deuteron beam on a beryllium target. The researchers also bombarded well-shielded sample targets of uranium-235 and plutonium-239, irradiating each sample for 30 seconds, going back and forth to get enough statistics for a relevant evaluation.

"The high-energy gamma rays essentially represent a unique signature that fission has occurred," says Prussin, "both because of their energies, which are above 3 MeV, and because of their temporal behaviors."

Researchers followed up the LBNL measurements with signature verification experiments at a new laboratory commissioned at Livermore for scanning cargo containers. The laboratory houses a 6-meter container provided by APL, one of the world's largest container transportation companies, and gives the researchers a realistic testing environment. In these experiments, they irradiated a 22-kilogram target of natural uranium with a beam from a 14-MeV neutron source. Their results confirmed the intensity of the signature in a realistic cargo-scanning configuration using 150 grams of HEU and a low-intensity source.

Good Results with Simulated Cargo

In studies using simulated cargo stacked around the target, the gamma rays produced were very intense, between 2.5 and 4 MeV. The neutron beam energy must be high enough to penetrate the cargo but low enough to avoid interfering activation. (The research indicates the neutron source should be between 5 and 8 MeV.) Although gamma radiation is 10 times stronger than delayed neutrons, it is weak but detectable, and high-resolution detectors are not required to measure it. Large arrays of low-resolution detectors, such as liquid scintillators, can be cheaply produced and easily deployed.

One question the team must resolve is what accelerator characteristics are required for practical field applications. "Accelerators that can give the appropriate deuteron beam energy intensity on the appropriate target can, in principle, be manufactured commercially and for a reasonable amount of funding," Prussin says. "We don't know that one has been constructed for the exact conditions we'll specify, and we may have some technical issues to address. But our requirement is not for a scientific system. What we will want is a much simpler device."

Meanwhile, the team wants to resolve some problems found when using Monte Carlo codes to mock up experiments and test them on the computer. "We are developing a method that seems likely to serve our purpose," says Prussin. Experiments on irradiation of uranium, which will be conducted at LBNL, are being designed to help the researchers understand how well the computational procedures represent the experimental data.

Simultaneously, efforts are moving forward to develop a large array of liquid scintillators that are sensitive to both neutron and gamma rays. As currently envisioned, the design includes a bank of 20 liquid scintillator–filled tubes spanning each side of the car wash.

Benefits of Liquid Scintillator

Liquid scintillator is a good candidate material for the cargo interrogation problem. It has a fast response time, and it can be inexpensively instrumented to scan a large volume of material, which helps to ensure that a large fraction of the particle flux emitted by the neutron-irradiated nuclear material will be detected. Livermore physicist Adam Bernstein, who leads the detector design team, says, "Neutrons and gamma rays create a 20-nanosecond pulse of blue light when they scatter in the medium, and this

fluorescent pulse can be detected in photomultiplier tubes." Such detectors can be used in various cargo detection and interrogation scenarios. For example, even with the neutron source off, the detector array may still be sensitive enough to scan cargo for some types of radioactive materials of concern.

The segmented array, which has a response time of about 100 nanoseconds or better, would indicate the location or spatial extent of radioactive material hidden in the cargo. "By establishing the geometric extent of the radioactive material," says Slaughter, "we can better differentiate cargo with small amounts of uranium distributed throughout from normal cargo with a small component of nuclear material hidden in it."

"The liquid scintillator project dovetails nicely with the Laboratory's mission," says Bernstein. "Livermore in general is a center for radiation detection because of nuclear weapons and other nuclear physics research." He adds that the liquid scintillator work is building on a detection technology that has been used for years in high-energy physics. "These types of detectors are often used in fundamental physics research, where we engage in neutrino physics and dark-matter searches, but not for practical applications such as fissile material detection. In this project, we're taking a technology that's a workhorse in high-energy physics and applying it in the real world."

Using liquid scintillators in such applications brings its own challenges for detector designers. "We have a lot of work to do in developing the algorithms for the gamma-ray signal that comes out of cargo containers," says Bernstein. "We want to process the signal in a different way than we do in a physics experiment where we don't have any time constraints and we can wait to obtain data. In this application, we have about a minute to decide whether the cargo container is suspicious or not."

APL, one of the world's largest container transportation companies, provided Livermore researchers with a 6-meter container, which gives them a realistic test environment in the container laboratory.

Keeping the false-positive and false-negative rates low is another technical issue facing the designers. "We want to optimize the signal-to-background ratio as best we can," says Bernstein, "and we'll have to establish the number of false positives that are acceptable. For example, if a few hundred cargo containers go through the car wash each day, a false-positive rate of 1 percent might be unacceptable because that could mean you stop the chain once a day to remove a container for closer inspection."

Another challenge is to develop a robust system, one that can work continually for months or years and that can be operated by people who are not experts in radiation detection. "People frequently underestimate that aspect of the development process," Bernstein says.

Members of the team built a small prototype of a 0.6-meter-tall detector, which they successfully tested. This spring, they are working with an array of four detectors, each 2 meters tall and 20 centimeters in diameter, and according to Bernstein, the team expects this testing to result in some iterations of the design. By the end of 2004, the team hopes to be working on a larger array that would cover one side of the car wash.

"By January or February 2005, we should have the full array," says Bernstein. "We most likely will build it at Livermore. While we're designing the prototype, we'll also try to make the system portable, so we can take it into the field—and possibly test it at a port."

Slaughter is hopeful that by 2005 the Laboratory team will add a commercial partner to develop a system that could eventually be deployed in the fight against global terrorism.

—Dale Sprouse

Key Words: cargo containers, gamma rays, highly enriched uranium (HEU), homeland security, liquid scintillator, nuclear materials, neutron generator, plutonium, terrorism, weapons of mass destruction.

For further information contact Dennis Slaughter (925) 422-6425 (slaughter1@llnl.gov).

Improved Algorithms
Speed It Up for Codes

HUGE computers, huge codes, complex problems to solve. The longer it takes to run a code, the more it costs. One way to speed things up and save time and money is through hardware improvements—faster processors, different system designs, bigger computers. But another side of supercomputing can reap savings in time and speed: software improvements to make codes—particularly the mathematical algorithms that form them—run faster and more efficiently.

Speed up math? Is that really possible? According to Livermore physicist Eugene Brooks, the answer is a resounding yes.

"Sure, you get great speedups by improving hardware," says Brooks, the deputy leader for Computational Physics in N Division, which is part of Livermore's Physics and Advanced Technologies (PAT) Directorate. "But the real bonus comes on the software side, where improvements in software can lead to orders of magnitude improvement in run times."

Brooks knows whereof he speaks. Working with Laboratory physicist Abraham Szöke and others, he has been instrumental in devising ways to shrink the running time of what has, historically, been a tough computational nut to crack: radiation transport codes based on the statistical or Monte Carlo method of calculation. (See the box on p. 18.) And Brooks is not the only one. Others around the Laboratory, including physicists Andrew Williamson, Randolph Hood, and Jeff Grossman, have come up with innovative ways to speed up Monte Carlo calculations using pure mathematics.

Monte Carlo Not Just for Gamblers

Radiation is energy on the move in the form of light rays or particles such as electrons. Thermal radiation consists of photons, which display characteristics of both high-speed particles and electromagnetic waves. The study of radiation transport deals with predicting and measuring how these photons move through matter. Put simply, thermal radiation transport is a calculational method that examines how heat moves around.

Such calculations are an important part of models that, for example, simulate stellar evolution or inertial confinement fusion experiments. For a mundane example of radiation transport in action, consider a radiant space heater such as those commonly found in homes and garages. Radiant heaters generate invisible infrared radiation that transfers heat not to the air—as convection heaters do—but directly to objects and people themselves. With a radiant space heater, people near the heater begin to feel warmer before the heater has had a chance to raise the temperature of the entire room.

Since the early days of modeling, thermal radiation transport codes have been used at Livermore to simulate how thermally generated photons interact with material. To set up a calculation using these codes, computer scientists divide a material into chunks called zones. Then they incorporate such data as the material's properties and the photons' initial energies, frequencies, and directions of travel. Time is also chopped into discrete steps. Once the problem is set up, the computer grinds through its calculations—step by step, photon by photon, zone by zone—to model how the photons, which transport the thermal energy, move through the material.

Modeling this thermal radiation phenomenon has always been difficult, Brooks notes. For example, a photon's mean free path—the average distance it travels before colliding with another photon—may be shorter than the length of the zone, or its mean free time may be shorter than the time step. These problems are frequently encountered in opaque systems such as the interior of stars. Scientists have developed several mathematical methods to solve such problems, including Monte Carlo radiation transport.

Tweaking for Results

Until 1970, the Monte Carlo method used to solve thermal radiation problems was very unstable, Brooks says. "In solving the equations over and over, proceeding through each time step, the numerical solutions had errors that grew over time. It wasn't a physical phenomenon, but a mathematical artifact that popped up in solving the problem on the computer."

In 1971, Joe Fleck and J. D. Cummings worked out an innovative method to dampen this mathematical instability, a scheme they called implicit Monte Carlo (IMC). In essence, they introduced the concept of effective scattering, wherein a fraction of the radiative energy absorbed during a time step is instantly reemitted in all directions before the next time step. In contrast, the more conventional Monte Carlo methods do not emit the absorbed photons until the following step—a process that over time causes the numerical instability. IMC was thus more stable and more accurate than traditional methods for certain situations. However, the effective scattering calculations required a lot of computer time to solve.

In the late 1980s, Fleck hired Brooks as a postdoctoral fellow to extend the IMC method so that it would be useful for lasers. Brooks developed a technique called symbolic IMC. "This technique removed the scattering problem," he says, "and, instead, it gave us a system of nonlinear mathematical equations, or a matrix, to solve."

Although the symbolic IMC method was faster and cleaner than the original IMC method, its nonlinear system still caused a problem: The noise in opaque materials required large numbers of Monte Carlo particles. Brooks and Szöke returned to this problem in 2003, to try to speed up the calculations. They found that the mathematical noise in the Monte Carlo system corresponds to what happens when a photon is absorbed in the zone in which it originates. This quick absorption of photons happens frequently in opaque materials. "As a result," says Brooks, "when we're modeling an opaque material, we often end up wasting a lot of time using computational power to solve a part of the problem that can easily be done with a pencil and paper."

The breakthrough came when the scientists realized that calculations aren't needed for all of the photons—only for the ones that escape one zone and are transported to the next. Szöke suggested subtracting the calculations of the photons being emitted and reabsorbed—a mathematical construct they called the difference formulation. "So far," Brooks says, "the difference formulation is working very well."

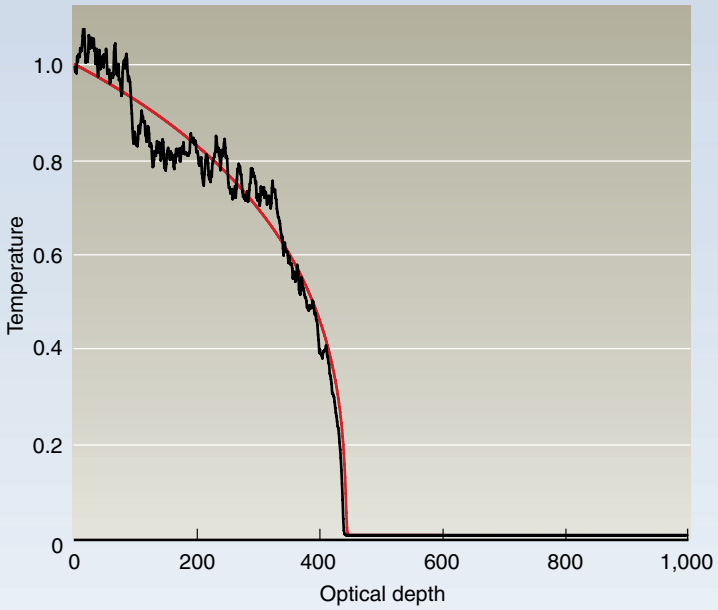
The initial test problem was a one-dimensional simulation of a thick material slab. The simulated slab was divided into many zones with various opacities and time steps. Using the difference formulation increased the algorithm processing speed by factors of up to 1 million, whereas using the older formulation on the massively parallel supercomputers improved speed by factors of 1,000 or so. The makers of supercomputers need not worry, however, because the difference formulation can be adapted to parallel computing, and, says Brooks, the demands of computer users for increased speed are insatiable.

Algorithms in Nanoscience

Mathematical improvements to Monte Carlo methods benefit other Livermore research areas besides astrophysics, including nanoscience. Williamson, Hood, and Grossman, who all work in PAT's Quantum Simulations Group, model systems with only 100 to 200 atoms to better determine their material properties. "At these sizes, quantum mechanical effects can change a material's properties," says Grossman. "For instance, shining laser light at a palm-size piece of silicon will cause the silicon to emit photons at a wavelength not visible to the human eye. If we shine the same laser light on a silicon quantum dot of 100 atoms (about 2 nanometers square), the dot emits visible light. What's more, the color of the emitted light—whether blue, red, or something in between—will depend on the size of the silicon chunk." (See *S&TR*, November 2003, pp. 4–10.)

Why do materials behave so oddly in such small quantities? The answer can be found in a solution of Schrödinger's equation, which describes the properties of an electron's wave function. In this world of the very small, the electron is treated as a wave, not as a particle. Solving Schrödinger's equation for one particle is simple enough to be done by hand. But as the number of electrons or particles grows, the calculation's complexity increases exponentially, so computers—and lots of computational time—are required to solve the problem.

One approach to these calculations is called the Quantum Monte Carlo (QMC) method. The QMC method uses random numbers to generate an approximate answer with an error bar that indicates the accuracy of the approximation. The smaller the error bar, the more accurate the approximation. To shrink the error bar, the code must choose more random numbers, which increases the program's processing time because the code runs more iterations. Ideally, the



A material's temperature is increased by the transport process of a thermal wave, which is propagating from left to right. The material was initially at 0.01 temperature units. At the start of the simulation, it was abruptly heated on the left side at a temperature of 1 unit. The black curve shows the results from a simulation using the standard formulation. The curve's jagged appearance is caused by the mathematical noise in the calculations. The red curve shows the results from a simulation using the difference formulation. This calculation was performed using the same run time on the same computer as the standard formulation. The Monte Carlo noise in the difference formulation is too small to be shown.

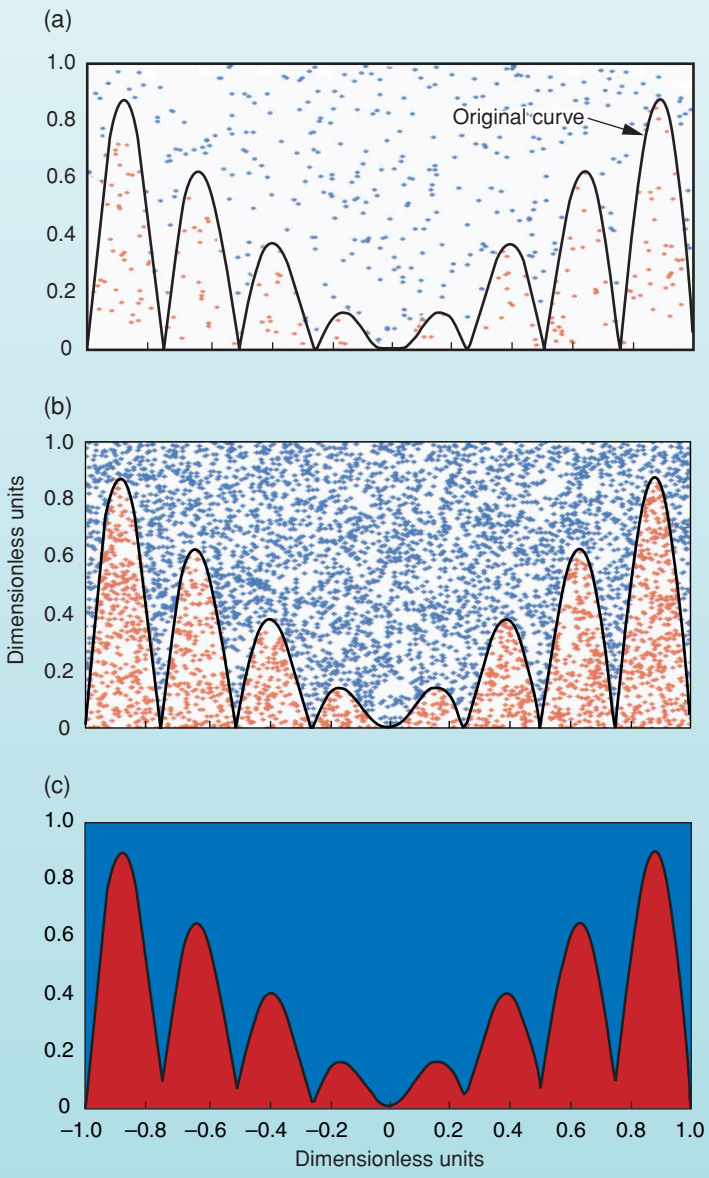
Monte Carlo Primer

In 1946, mathematician Stanislaw Ulam named a set of statistical problem-solving methods "Monte Carlo." The code itself was created at Los Alamos National Laboratory during the Manhattan Project, and the first Monte Carlo calculations were performed in 1948 on the ENIAC, the world's first electronic digital computer. Monte Carlo methods use sequences of random numbers to perform computer simulations. Every simulation is based on events that happen randomly, so the outcome of a calculation is not always absolutely predictable—much like the throw of a dice or turn of a card. Monte Carlo is used routinely in diverse fields, including simulations of radiation transport in Earth's atmosphere and esoteric subnuclear processes in high-energy physics experiments. The difference between Monte Carlo, the method, and Monte Carlo, the gaming capital, is that the method's "game" involves a physical system rather than a game of chance, and its outcome is not a pot of money or stack of chips, but rather the solution to a problem.

Simple Monte Carlo at Work

A simple example of the Monte Carlo method is shown in the figure at right, where random numbers are used to calculate the area under a curve as a fraction of the rectangular box encompassing the curve. The original curve is enclosed within a rectangle, and points within the rectangle are chosen at random. The number of points under the curve is then determined as a fraction of the total points chosen. Because the total area of the enclosing rectangle is known, the ratio of the points under the curve to the total points approximates the fraction of the area lying under the curve. As more points are chosen, the approximation becomes more exact.

For example, when only 500 points are chosen, the calculation estimates the area under the curve as 69.6 percent of the total area within the rectangle. But the accuracy of this estimate may be off by as much as 6 percent. Accuracy improves when more random numbers are chosen. With 5,000 points, the area under the curve is estimated to be 63.96 percent, and the error shrinks to 0.29 percent. With 500,000 points, the area is 63.53 percent with an error of 0.13 percent.



A computer code using Monte Carlo calculations can estimate the area under a curve as a fraction of the rectangular box that encompasses the curve. (a) When the code generates 500 random points, the area under the curve is estimated to be 69.6 percent of the rectangle, but the error is 5.9 percent. (b) With 5,000 points, the area is estimated to be 63.96 percent, and the error shrinks to 0.29 percent. (c) With 500,000 points, the area is 63.53 percent with an error of 0.13 percent.

error bar should be smaller than the differences being measured in the calculation. For example, if scientists want to determine whether the light emitted by a particular quantum dot will be blue or red, they set the code to calculate an answer that's accurate enough—that has an error bar small enough—to differentiate between the opposite ends of the visible spectrum.

In determining whether an answer can be trusted, scientists can either run the simulation until the error bar is small enough or compare the results with accuracy benchmarks established in physical experiments. "In nanoscience, experiments are difficult to do because of the extremely small scales," says Grossman, "so the ability to use highly accurate benchmark methods such as QMC are quite valuable."

Until recently, however, QMC was only practical when looking at systems composed of small numbers of atoms. "It was a scaling issue," says Grossman. "For instance, if it took 10 minutes for QMC to run a problem with 10 atoms, then running that same problem with 100 atoms required 10,000 minutes—or nearly a week of computational time."

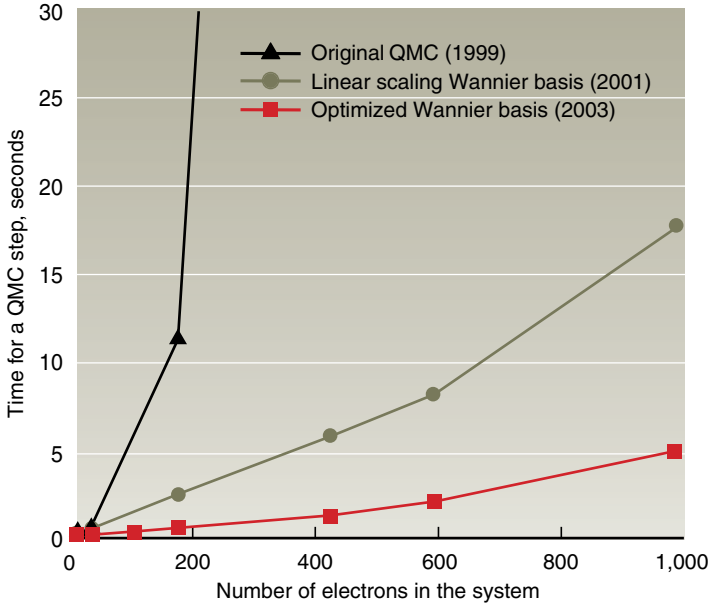
To solve the scaling problem, Grossman, Williamson, and Hood applied a novel mathematical approach called the Wannier basis to the QMC algorithm. Essentially, they performed a mathematical transformation, taking a problem that was difficult to solve and transforming it into a domain where it was easier to solve. For example, one common mathematical transformation is using logarithms, a method for converting difficult multiplication problems into simpler addition problems. Another is performing a Fourier transform, to change the wave of a complex electrical signal into simpler sine and cosine waves.

In the original QMC algorithm, the time needed to solve a problem scaled as the cube of the number of atoms involved. Applying the Wannier transformation to QMC produces an algorithm that scales linearly. As a result, the 100-atom system, which previously took a week to process, now requires only 100 minutes.

Williamson is working with Livermore physicist Fernando Reboredo to optimize these Wannier transformations. "We're using nonorthogonal basis functions, which speed up the code another five times," says Williamson. "That increase reduces the run time for the 100-atom system to only 20 minutes. The code also uses eight times less memory, so we can study much larger nanoscience problems."

Math That Makes a Difference

Even as supercomputing hardware improves, computational scientists, physicists, and others look for better ways to increase the speed of their calculations. Each advance in trimming the time to run a code opens the possibility for simulating a process in more detail and for running multiple simulations in the same amount of time—or even less time—than had been required to process only one.



With a mathematical transformation called the Wannier basis, the number of electrons in a Quantum Monte Carlo (QMC) simulation can be increased without a prohibitive increase in the calculation's run time.

"Each step forward," says Brooks, "is based on the work that was done before. The advances often happen when people have the opportunity to come together and think differently. It's the collision of people and ideas—through hard work and sudden insights—that leads to these new mathematical constructs, which, in turn, yield faster and in some cases more accurate predictions of phenomenon. In a way, these innovations owe much to serendipity, a lucky roll of the dice—it's Monte Carlo in the scientific realm."

—Ann Parker

Key Words: algorithm, difference formulation, implicit Monte Carlo (IMC) method, Monte Carlo, nanoscience, quantum dots, Quantum Monte Carlo (QMC) method, thermal radiation transport, Wannier basis.

For further information contact Eugene Brooks (925) 423-7341 (eugenebrooks@llnl.gov) or Jeff Grossman (925) 423-6991 (grossman3@llnl.gov).

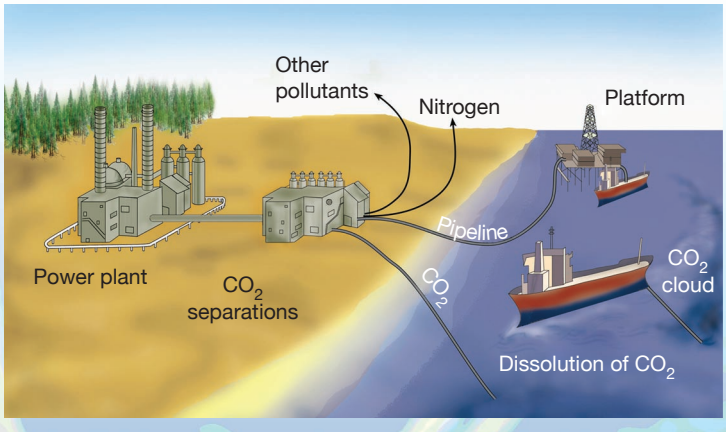
The Siren Call of the Seas

Sequestering Carbon Dioxide

MOST experts now agree: increased emissions of greenhouse gases, especially carbon dioxide, are responsible for the overall warming of our planet. Yet, reversing the rate of these emissions, or even holding it steady, appears to be a nearly impossible task. In the 20th century alone, the human population quadrupled, and primary power consumption increased 16-fold. During that same time, atmospheric carbon dioxide increased from about 275 to 370 parts per million—and demand for power continues to grow.

Scientists cannot fully predict the future effects of carbon dioxide buildup. However, most of them agree that serious environmental consequences are possible unless the management of carbon dioxide emissions improves.

The burning of fossil fuels—coal, oil, and gas—is expected to be the main source of energy for the foreseeable future. For instance, according to the International Atomic Energy Agency, fossil fuels will account for almost all new electric power generating capacity during the next 20 years: 78 percent for the developing world, up to 97 percent for transition economies, and 89 percent for the developed world. Doing away with all of the carbon dioxide that results from power production is unrealistic. Instead, scientists are focused on finding methods to stabilize the amount of carbon dioxide being added to the atmosphere.



One possible method for stabilizing the amount of carbon dioxide (CO_2) in the atmosphere is to inject it into the deep ocean, either from shore stations or from tankers at sea. (Reprinted courtesy of Lawrence Berkeley National Laboratory, Earth Sciences Division. Artist: Raine Reen.)

One approach being studied at Livermore is to sequester carbon dioxide—that is, capture the carbon and store it for long geologic time periods.

Carbon dioxide can be stored in several ways. For example, compressed carbon dioxide can be injected into geologic formations such as depleted oil and gas fields or saline aquifers (see *S&TR*, December 2000, pp. 20–22), or it can be injected into the oceans. Oceans absorb carbon dioxide naturally in ongoing processes that are very slow. However, the oceans' capacity for carbon dioxide is quite large. They already take up one-third of the carbon emitted by human activity, which is about 2 billion metric tons each year.

In July 1999, the Department of Energy established the Ocean Carbon Sequestration Research Program to investigate the feasibility, effectiveness, and environmental acceptability of ocean carbon sequestration. "We evaluate the underlying science of various options," says atmospheric scientist Ken Caldeira, who leads the ocean carbon storage research at Livermore. "We look at the different proposals for increasing ocean carbon storage and present information to the policy makers who determine the nation's course of action in this area."

Caldeira is also leading the process to review ocean carbon storage options for the Intergovernmental Panel on Climate Change. This review will form the basis for international negotiations on the treatment of purposeful ocean carbon storage under the United Nations Framework Convention on Climate Change.

Sink It in the Ocean?

Two ocean carbon strategies are being considered. One is to inject carbon dioxide directly into the deep sea, and the other is to fertilize the ocean with iron, which will increase its uptake of atmospheric carbon dioxide.

Direct injection involves separating carbon dioxide from the flue gas produced by power plants, compressing and liquefying it, and then pumping it into the ocean. (See the figure at left.) If the injection site is deep enough, carbon dioxide will sink and perhaps form a "lake" at the bottom of the ocean. One concern about this approach, says Caldeira, is that the pH level of such a lake would make the deep ocean environment more acidic. However, the increased acidity will affect the ocean whether carbon is injected or remains in the atmosphere—it's just a matter of what part of the ocean will be most affected.

"If we continue consuming fossil fuels without doing anything at all," Caldeira says, "the ocean—particularly its upper layer—will become more acidic than it has been in millions of years. That change is bound to affect corals and other marine life near the surface of the ocean. By piping it down deep, we might protect this biosystem to some extent, but how the increased acidity will affect the lower depths of the ocean has yet to be determined."

The other major approach to ocean sequestration involves fertilizing the ocean with iron. Adding nutrients such as iron to the surface of the ocean can stimulate the growth of phytoplankton, which would take up additional carbon from the atmosphere as well. When these plants and the animals that eat them reach the end of their lifecycles and die, they—and the carbon inside them—would eventually drift down into the ocean's depths. Carbon dioxide from the atmosphere would then enter the surface ocean to replace some of the carbon that sinks.

But Will It Work?

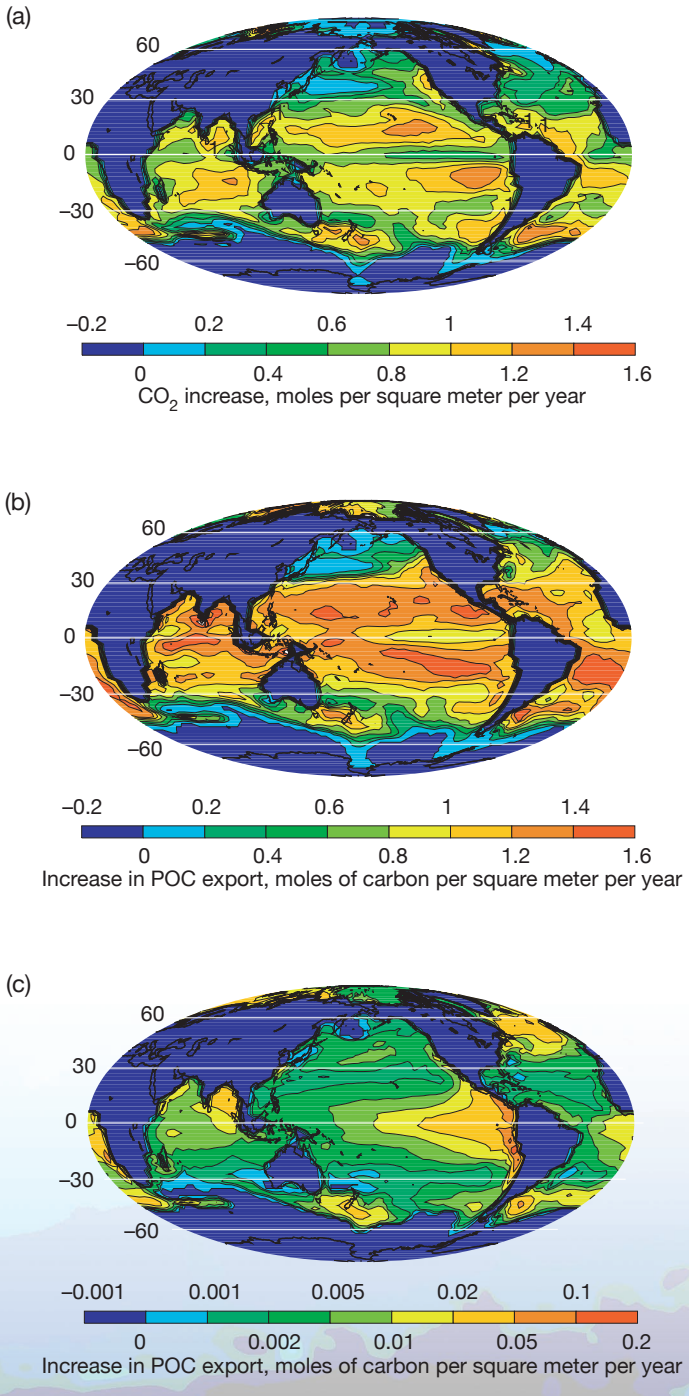
To evaluate the consequences and effectiveness of various options, Caldeira and his colleagues simulated different scenarios using the Livermore ocean general-circulation model. For example, simulations of iron fertilization of the oceans in the Southern Hemisphere initially showed that almost 8 billion tons of carbon would be absorbed by the ocean each year. Yet, after 500 years of continuous fertilization, the net increase in absorption would be less than 1 billion tons of carbon per year. (See the figure at right.)

Caldeira explains, "A couple of things happen to make this net absorption so low. First, the previously sequestered carbon dioxide does eventually leak back out of the ocean, although the leakage rate is most rapid in the first years." Carbon detritus that sinks to layers of constant density that are poorly ventilated to the atmosphere will stay in the ocean a long time.

Another issue arises with the bloom of marine plant life and the availability of other nutrients. "The models indicate that, eventually, other macronutrients become depleted even as we add iron," says Caldeira. "When that happens, the bloom falters, and the organisms are no longer taking up as much carbon as they did in the beginning."

Many unknowns remain, and much is yet to be worked out. "There are pros and cons to this approach," Caldeira says, "but it might be an effective low-cost technique, even with the leakage. Most living things would probably grow better, and the results could be monitored to avoid environmental surprises. However, at best, it's only a partial solution to the problem, and it would involve ecosystem management on an unprecedented scale."

The team also examined different facets of the direct injection technique and its variations using the same ocean model. Caldeira, Mike Wickett of the Center for Applied Scientific Computing, and Philip Duffy of the Climate and Carbon Cycle Modeling Group



Simulations of the iron fertilization process after 1 year show a dramatic increase in (a) the flux of carbon dioxide (CO_2) from the atmosphere to the ocean and (b) the sedimentary export of particulate organic carbon (POC) from the surface ocean. However, after 500 years, (c) POC export has greatly diminished.

used one-dimensional box-diffusion models and three-dimensional simulations to examine what happens over time when carbon dioxide is injected at different depths in the ocean. Injections were simulated at 800, 1,500, and 3,000 meters for 100 years near the Bay of Biscay, New York City, Rio de Janeiro, San Francisco, Tokyo, Jakarta, and Bombay. The team found that deeper injection led to longer sequestration, with the specific location of injection having less effect on sequestration time. Injection at a depth of 3,000 meters sequestered carbon from the atmosphere for several centuries, but shallower injections were less effective.

In a more recent project, Caldeira and Wickett simulated the direct injection of fossil-fuel carbon so they could assess the relative effectiveness of different injection sites and depths. Again, using the ocean general-circulation model, they injected carbon dioxide continuously at a rate of 0.1 million tons per year at 710 and 3,025 meters off the coasts of New York and San Francisco. At both sites, carbon escapes the ocean more slowly if it is injected more deeply. The highest fluxes of injected carbon escaping the ocean occur far from the injection site. For both the shallow and deep injection depths, carbon escapes the ocean more slowly for the San Francisco site than for the New York site.

The specific whys and wherefores of these results have much to do with circulation systems of the different oceans as well as the viscosity, salinity, and density of the ocean water at various depths and locations. For instance, the simulations showed that large-scale advective processes may be more important in bringing deep water to the surface in the Atlantic basin than in the Pacific basin, so carbon escapes more readily from the New York site.

In another project using the same model, Caldeira and Wickett compared the changes in pH when carbon dioxide is injected into the ocean and released to the atmosphere. They simulated the release of 7 petagrams of carbon annually (1 petagram is 1 billion metric tons or 1,000 billion kilograms) for 1,000 years into the atmosphere and into the ocean at 3 kilometers. They found that, whether carbon dioxide is released to the atmosphere or in the ocean, eventually, about 80 percent of it ends up in the ocean in a form that will make the ocean more acidic. However, with ocean injection, the problem of acidity is moved from the ocean surface to the deep. Previous studies showed that unless carbon dioxide is converted to some other form before injection, it will eventually make its way back into the atmosphere after diffusion or ocean circulation returns it to the ocean surface.

Limestone May Help

In research funded by Livermore's Laboratory Directed Research and Development Program, Livermore geochemist Kevin Knauss worked with Greg Rau of the University of California at Santa Cruz to address the pH problem. One solution may be to use common limestone in a technique called enhanced carbonate dissolution. This process involves hydrating carbon dioxide from power plant flue gas with water to produce a carbonic acid solution. The solution is then mixed with crushed limestone, which neutralizes the carbon dioxide by converting it to a calcium bicarbonate solution that can be released into the ocean. This process converts the carbon dioxide to a form that does not readily exchange with the atmosphere and that causes a less drastic change to the ocean's pH. The process occurs in nature through carbonate weathering, but at a much slower pace than envisioned in this enhanced version.

According to Rau, the carbonate dissolution process also might expand the capacity of the ocean to store carbon dioxide and minimize the amount of carbon escaping to the atmosphere. Another benefit is that the process would add calcium and bicarbonate to the ocean, which would enhance the growth of corals and other calcifying marine organisms.

Data for Deciding the Future

But what if no system is used to mitigate the release of carbon dioxide? Caldeira and Wickett also modeled the repercussions from that approach. The model incorporated historical and geologic data on carbon dioxide and emissions generated from the scenario set by the Intergovernmental Panel of Climate Change for the years 2000 to 2100. In addition, they explored the consequences of burning the remaining fossil-fuel resources during the next several centuries. The modeling results indicated that, unabated, carbon dioxide emissions over the coming centuries could produce changes in ocean pH that are greater than any experienced in the past 300 million years.

Caldeira adds that the research team is not responsible for making a policy decision. "Whether the decision is to do nothing, to do one thing, or to try a range of techniques, it is not our choice to make," he says. "Our role is not to be an advocate or back any particular options—one way or another. Our role is to provide the underlying science so that policy makers can make informed decisions."

—Ann Parker

Key Words: carbonate dissolution, carbon dioxide sequestration, Center for Research on Ocean Carbon Sequestration, fossil fuels, iron fertilization, ocean general-circulation model, ocean sequestration.

For further information contact Ken Caldeira (925) 423-4191 (caldeira2@llnl.gov).

Each month in this space we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Saccharide Sensing Molecules Having Enhanced Fluorescent Properties

Joe H. Satcher, Jr., Stephen M. Lane, Christopher B. Darrow, Douglas R. Cary, Joe Anh Tran
U.S. Patent 6,673,625 B2
January 6, 2004
This invention provides formulae for fluorescent compounds with properties that make them well suited for use in analyte sensors such as saccharides. These properties include favorable excitation and emission wavelengths and fluorescence lifetimes as well as photostability, enhanced aqueous solubility, and temperature and pH sensitivity. The compound has an aryl or a substituted phenyl botonic acid that acts as a substrate recognition component, a fluorescence switch component, and a fluorophore. The fluorescent compounds are excited at wavelengths greater than 400 nanometers and emit at wavelengths greater than 450 nanometers, which is advantageous for optical transmission through skin. The fluorophore is typically selected from transition metal–ligand complexes and thiazine, oxazine, oxazone, or oxazine-one as well as from anthracene compounds. The fluorescent compound can be immobilized in a glucose-permeable biocompatible polymer matrix and implanted under the skin.

Parallel Object-Oriented Data Mining System

Chandrika Kamath, Erick Cantu-Paz
U.S. Patent 6,675,164 B2
January 6, 2004
A data mining system uncovers patterns, association, anomalies, and other statistically significant structures in data. When data files are read and displayed, objects in the files are identified, and relevant features of the objects are extracted. Patterns among the objects are recognized based on the features. Data from the Faint Images of the Radio Sky at Twenty Centimeters (FIRST) sky survey were used to search for bent doubles. This test was conducted on data from the Very Large Array in New Mexico, which seeks to locate a special type of quasar—a radio-emitting stellar object—called bent doubles. The FIRST survey has generated more than 32,000 images of the sky to date. Each image is 7.1 megabytes, yielding more than 100 gigabytes of image data in the entire data set.

Manifold Free Multiple Sheet Superplastic Forming

John W. Elmer, Robert L. Bridges
U.S. Patent 6,677,011 B2
January 13, 2004
Fluid-forming compositions in a container attached to enclosed adjacent sheets are heated to relatively high temperatures to generate fluids (gases) that inflate the sheets. Fluid rates to the enclosed space between the sheets can be regulated by the canal from the container. Inflated articles can be produced by a continuous, rather than batch-type process.

Thin Film Transistors on Plastic Substrates

Paul G. Carey, Patrick M. Smith, Thomas W. Sigmon, Randy C. Aceves
U.S. Patent 6,680,485 B1
January 20, 2004
A process for forming thin-film transistors (TFTs) on plastic substrates, which replaces standard TFT fabrication techniques, uses sufficiently lower processing temperatures so that inexpensive plastic substrates may be used in place of standard glass, quartz, and silicon wafer–based substrates. The silicon-based TFT produced by the process includes a low-temperature substrate that is incapable of withstanding sustained processing temperatures greater than about 250°C; an insulating layer on the substrate; a layer of silicon on the insulating layer that has sections of doped silicon, undoped silicon, and polysilicon; a gate dielectric layer on the layer of silicon; a layer of gate metal on the dielectric layer; a layer of oxide on sections of the silicon layer and the gate-metal layer; and metal contacts on sections of the silicon and gate-metal layers to define source, gate, and drain contacts as well as interconnects.

Single-Fiber Multi-Color Pyrometry

Ward Small IV, Peter Celliers
U.S. Patent 6,682,216 B1
January 27, 2004
This invention is a fiber-based multicolor pyrometry set up for real-time noncontact temperature and emissivity measurement. The system includes a single optical fiber to collect radiation emitted by a target; a reflective rotating chopper to split the collected radiation into two or more paths while modulating the radiation for lock-in amplification; at least two detectors, possibly of different spectral bandwidths, with or without filters to limit the wavelength regions detected; and optics to direct and focus the radiation onto the sensitive areas of the detectors. A computer algorithm is used to calculate a target's true temperature and emissivity based on blackbody calibrations. The system components are enclosed in a light-tight housing, with a fiber extending outside to collect the radiation. Radiation emitted by the target is transmitted through the fiber to the reflective chopper, which either allows the radiation to pass straight through or reflects the radiation into one or more paths. Each path includes a detector with or without filters and corresponding optics to direct and focus the radiation onto the active area of the detector. The signals are recovered using lock-in amplification. Calibration formulas for the signals obtained using a blackbody of known temperature are used to compute the target's true temperature and emissivity. The temperature range of the pyrometer system is determined by the spectral characteristics of the optical components.

Glucose Sensing Molecules Having Selected Fluorescent Properties

Joe H. Satcher, Jr., Stephen M. Lane, Christopher B. Darrow, Douglas R. Cary, Joe Anh Tran
U.S. Patent 6,682,938 B1
January 27, 2004
An analyte-sensing fluorescent molecule that uses intramolecular electron transfer is designed to exhibit selected fluorescent properties in the presence of analytes such as saccharides. The selected fluorescent properties include excitation wavelength, emission wavelength, fluorescence lifetime, quantum yield, photostability, solubility, and temperature or pH sensitivity. The compound has an aryl or a substituted phenyl boronic acid that acts as a substrate recognition component, a fluorescence switch component, and a fluorophore. The fluorophore and switch component are selected so that the free energy for electron transfer is less than about 3.0 kilocalories per mole. Fluorescent compounds are excited at wavelengths greater than 400 nanometers and emit at wavelengths greater than 450 nanometers, which is advantageous for optical transmission through skin. The fluorophore is typically selected from transition metal–ligand complexes and thiazine, oxazine, oxazone, or oxazine-one as well as from anthracene compounds. The fluorescent compound can be immobilized in a glucose-permeable biocompatible polymer matrix and implanted under the skin.

Movement of Particles Using Sequentially Activated Dielectrophoretic Particle Trapping

Robin R. Miles
U.S. Patent 6,685,812 B2
February 3, 2004
Manipulation of DNA and cells or spores using dielectrophoretic (DEP) forces to prepare samples for polymerized chain reaction– (PCR-) based assays for various applications. This manipulation is accomplished by moving particles using sequentially activated DEP particle trapping. DEP forces induce a dipole in particles, so the particles can be trapped in nonuniform fields. The particles can be trapped in the high-field-strength region of one set of electrodes. By switching off this field and switching on an adjacent electrode, particles can be moved down a channel with little or no flow.

Highly-Basic Large-Pore Zeolite Catalysts for NO_x Reduction at Low Temperatures

Bernardino M. Penetrante, Raymond M. Brusasco, Bernard T. Merritt, George E. Vogtlin
U.S. Patent 6,685,897 B1
February 3, 2004
A high-surface-area (greater than 600 square meters per gram), large-pore (diameter greater than 0.65 nanometer), basic zeolite with a structure such as an alkali metal cation-exchanged Y-zeolite is used to convert nitrogen oxides (NO_x) contained in an oxygen-rich engine exhaust to nitrogen and oxygen. Preferably, the invention relates to a two-stage method and apparatus for NO_x reduction in an oxygen-rich engine exhaust, such as diesel engine exhaust, that includes a plasma oxidative stage and a selective reduction stage. The first stage uses a nonthermal plasma treatment of NO_x gases in an oxygen-rich exhaust and is intended to convert nitric oxide to nitrogen dioxide in the presence of oxygen and added hydrocarbons. The second stage uses a lean-NO_x catalyst including the basic zeolite at relatively low temperatures to convert the nitrogen dioxide to environmentally benign gases such as nitrogen, carbon dioxide, and water.

Aerosol Sampling System

Donald A. Masquelier
U.S. Patent 6,688,187 B1
February 10, 2004
A system for sampling air and collecting particulate of a predetermined range of particle sizes. A low-pass section has an opening that is sized to gather the air but exclude particles larger than the sample particles. An impactor section connected to the low-pass section separates the air flow into either a bypass air flow, which does not contain the sample particles, or a product air flow, which does contain the sample particles. A wetted-wall cyclone collector, connected to the impactor section, receives the product air flow and traps the sample particles in a liquid.

Awards

The **Federal Laboratory Consortium** (FLC) has given **Lawrence Livermore** and **ORTEC Products** of Oak Ridge, Tennessee, a **2004 Excellence in Technology Transfer Award** for the public–private partnership that helped speed critical homeland security technology to the marketplace. In late 2002, the U.S. Department of Energy's National Nuclear Security Administration (NNSA) identified an urgent national need for a portable, easy-to-use radiation detector that could accurately screen for dangerous radioisotopes in luggage or shipping containers and report its results on the spot. Livermore researchers had built and demonstrated such a detector, called RadScout, but they needed an industrial partner to make it commercially available. Working to meet NNSA's request, the Laboratory found a partner and, by the end of 2002, had completed negotiations with ORTEC Products to develop RadScout into a commercial product, now called Detective.

RadScout was created by a team of electrical and mechanical engineers, physicists, vacuum specialists, and prototype manufacturers from Livermore's Engineering; Defense and Nuclear Technologies; and Nonproliferation, Arms Control, and International Security directorates. The Laboratory's Industrial Partnership and Commercialization Office handled the licensing negotiations with ORTEC.

The FLC, a nationwide network of more than 600 national laboratories from 16 federal agencies, recognizes outstanding work in transferring technology from the laboratories to the public and private sectors.

Tammy Jernigan, the principal deputy associate director of Physics and Advanced Technologies, was named the **2004 Outstanding Woman of the Year** in the science category by the **Alameda County Women's Hall of Fame**. Jernigan joined the Laboratory in 2001. Prior to that, she worked for the National Aeronautics and Space Administration (NASA). Jernigan became an astronaut in July 1986 and is a veteran of five space shuttle missions.

The Alameda County Women's Hall of Fame was established in October 1993 to recognize outstanding women in the California county for their achievements and contributions to the county and its citizens.

Abstracts

Life at the Nanoscale

Researchers at Livermore's BioSecurity and Nanosciences Laboratory (BSNL) are discovering new methods to detect, identify, image, and understand pathogens such as viruses, bacteria, and their spores. The research findings are helping to fight bioterrorism and improve human health. They also are contributing to the Department of Energy's Genomics:GTL Program, the follow-on effort to the Human Genome Project. Principal research areas are protein analysis and systems biology, bioaerosol science, molecular recognition chemistry, physical and chemical pathogen signatures (detection techniques), nanofabrication of devices, and cellular- and molecular-scale measurements. The researchers use powerful imaging techniques such as atomic force microscopy, confocal optical microscopy, and nano secondary-ion mass spectrometry as well as biomass spectrometry. The BSNL researchers, who are experts at synthesizing nanostructured materials, are studying single molecules—an emphasis that differs greatly from traditional biological research, which focuses on large quantities of material and then infers the role of individual molecules.

Contact:

Jim De Yoreo (925) 423-4240 (deyoreo1@llnl.gov).

Screening Cargo Containers to Remove a Terrorist Threat

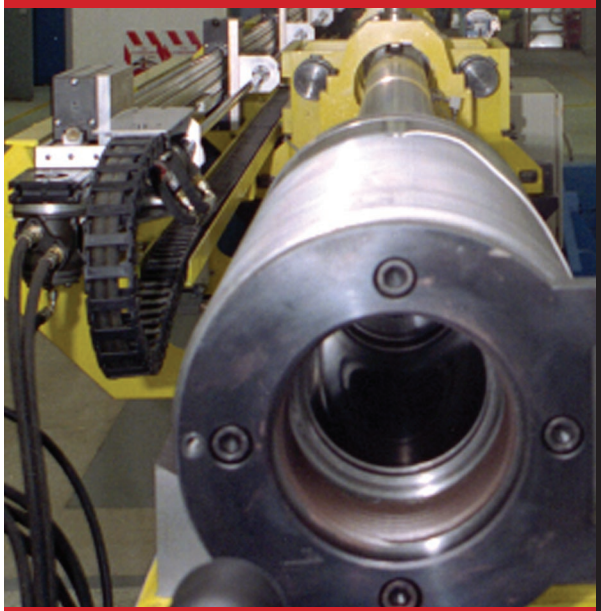
Livermore researchers are building on the Laboratory's expertise in radiation science and detection to prevent and deter terrorists from concealing nuclear weapons and materials inside cargo containers shipped to the U.S. Some 48 million cargo containers move between the world's seaports annually. More than 6 million of these containers enter U.S. seaports, but only about 2 percent are opened and inspected. The research team is developing a system to search for nuclear materials in suspect cargoes when questions are raised by other container screening procedures. The system's key components are a neutron generator and an array of liquid scintillation detectors, configured to look much like a car wash. A truck carrying a container of suspicious cargo would be towed through the array, and the container would be bathed in neutrons. The detectors would pick up the gamma-ray signature generated by any fissile material interacting with the neutrons. The researchers' goal is to develop a system that can complete a cargo-container scan within 1 minute, searching for small quantities of nuclear materials such as plutonium and highly enriched uranium.

Contact:

Dennis Slaughter (925) 422-6425 (slaughter1@llnl.gov).

U.S. Government Printing Office: 2004/683-056-70058

Plutonium at Extreme Conditions



A new two-stage gas gun at the Nevada Test Site helps scientists study how plutonium behaves under extreme pressures and temperatures.

Also in June

• As supercomputing settles into the terascale regime, simulations reveal insights about the physics of weapons in the nation's stockpile.

• Livermore scientists refine the techniques for analyzing the first dust samples collected from a comet.

• A new cleanup program at Livermore's Contained Firing Facility maintains beryllium exposure well below established standards.

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